Lect 6 Interacting electron gas: — Screening, collective modes

*) Screening:

$$H = \sum_{k\sigma} \varepsilon(k)\, C^{+}_{k\sigma} C_{k\sigma} + \frac{1}{2V} \sum_{kk'q} V(q)\, C^{+}_{k+q\sigma} C^{+}_{k'-q\sigma'} C_{k'\sigma'} C_{k\sigma}$$

consider an external perturbation $H_{ex}(t) = \frac{1}{V} \sum_{q} V_{ex}(q,t)\, \rho(-q,t)$

where $\rho(q) = \sum_{k\sigma} C^{+}_{k\sigma} C_{k-q,\sigma}$ ← density operator

From the linear response

$$\delta\rho(q,t) = -\int_{-\infty}^{+\infty} dt'\, \chi_{ret}(q, t-t')\, V_{ex}(t')$$

or $\delta\rho(q,\omega) = -\chi_{ret}(q,\omega)\, V_{ex}(q,\omega)$, where

$$\chi_{ret}(q,\omega) = \frac{i}{\hbar}\int_{-\infty}^{+\infty} dt\, e^{i(\omega+i\eta)t}\, \theta(t) \langle \cdot\cdot | \rho(q,t)\, \rho(-q,0) | \cdot\cdot \rangle$$

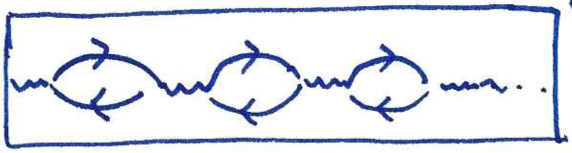
$\langle | \; | \rangle$ means the ground state average at zero temperature or thermal average at finite ~~temperature~~.

$\chi_{ret}(q,\omega)$ is the response for inter-acting systems. We can use the idea of self-consistency to appoximate as

response of the free electron system

$$\delta\rho(q,\omega) = -\chi_0(q,\omega)\, V_{tot}(q,\omega)$$

$$\delta\rho(q,\omega) = -\chi_0(q,\omega)\left[V_{ex} + V_{ind} \right]$$



$$-\nabla^2 V_{ind} = 4\pi e^2 \delta\rho(q,\omega) \Rightarrow V_{ind} = \frac{4\pi e^2}{q^2}\delta\rho(q,\omega)$$

$$= v(q)\,\delta\rho(q,\omega)$$

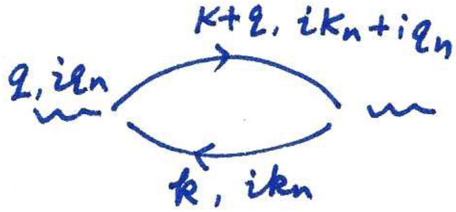
$$\Rightarrow \delta\rho(q,\omega) = \frac{-\chi_0(q,\omega)}{1 + v(q)\chi_0(q,\omega)} V_{ext}(q,\omega)$$

$$V_{tot} = V_{ex} + V_{ind} = \frac{1}{1 + v(q)\chi_0(q,\omega)} V_{ex}(q,\omega)$$

$$\Rightarrow \boxed{\varepsilon(q,\omega) = 1 + \frac{4\pi e^2}{q^2}\chi_0(q,\omega)} \leftarrow \text{dielectric function}$$

$$\chi^0_{ret}(q,\omega) = \frac{i}{\hbar}\int_{-\infty}^{+\infty} dt\ \theta(t)\ \langle|\rho(q t)\,\rho(-q,0)|\cdots\rangle.$$

→ Matsubara representation



$$\chi^0(q,iq_n) = \frac{1}{V}\int_0^\beta d\tau\ e^{i\omega\tau}\langle T_\tau|\rho(q,\tau)\,\rho(-q,0)|\rangle$$

$$= \frac{-2}{V\beta}\underset{\swarrow\text{spin}}{\sum_{k,\sigma}}\sum_{ik_n} \mathcal{G}^0(k+q, ik_n+iq_n)\,\mathcal{G}^0(k, ik_n)$$

Ex: frequency summation: define $S = \frac{+1}{\beta}\sum_{ik_n}\frac{1}{ik_n+iq_n-\varepsilon_{k+q}}\frac{1}{ik_n-\varepsilon_k}$

$$I = \lim_{R\to\infty}\oint\frac{dz}{2\pi i} f(z)\frac{1}{e^{\beta z}+1} = 0, \text{ where } f(z)$$

$$= \frac{1}{iq_n + z - \varepsilon_{k+q}}\frac{1}{z-\varepsilon_k}$$

$$\Rightarrow \ -\frac{1}{\beta}\sum_n f(i\omega_n) + \sum_i \mathrm{Res}\left(\frac{f(z)}{e^{\beta z}-1}\right)\Big|_{z=z_i} = 0$$

$$\Rightarrow S = \frac{1}{-iq_n + \varepsilon_{k+q} - \varepsilon_k}\,\frac{1}{e^{\beta(\varepsilon_{k+q}+iq_n)}+1} + \frac{1}{iq_n + \varepsilon_k - \varepsilon_{k+q}}\,\frac{1}{e^{\beta\varepsilon_k}+1}$$

$$= \frac{n_f(\varepsilon_k) - n_f(\varepsilon_{k+q})}{iq_n - (\varepsilon_{k+q} - \varepsilon_k)}$$

$$\Rightarrow \chi^0(q, iq_n) = -2\int \frac{d^3\vec{k}}{(2\pi)^3}\,\frac{n_f(\varepsilon_k) - n_f(\varepsilon_{k+q})}{iq_n - (\varepsilon_{k+q} - \varepsilon_k)}$$

Real frequency:

$$\chi^0(q, \omega + i\eta) = -2\int \frac{d^3\vec{k}}{(2\pi)^3}\,\frac{n_f(\varepsilon_k) - n_f(\varepsilon_{k+q})}{\omega - (\varepsilon_{k+q} - \varepsilon_k) + i\eta}$$ ← Lindhardt response

at small q-limit : $q \ll k_f$

$$n_f(\varepsilon_k) - n_f(\varepsilon_{k+q}) = -\frac{\partial n}{\partial \varepsilon}(\varepsilon_{k+q} - \varepsilon_k) = \delta(\varepsilon - \mu)\,\vec{v_F}\cdot\vec{q}$$

$$\chi^0(q, \omega + i\eta) = N_0 \int \frac{d\Omega}{4\pi}\,\frac{-\cos\theta\, v_F q}{\omega - v_F q\cos\theta + i\eta}$$, where $N_0 = \frac{2}{(2\pi)^3}\int \underbrace{k^2 dk \int d\Omega}_{\delta(\varepsilon-\mu)}$

$$= N_0\left[1 - \int \frac{d\Omega}{4\pi}\,\frac{s}{s - \cos\theta + i\eta}\right]$$, where $s = \frac{\omega}{v_F q}$.

$$\mathrm{Re}\int \frac{d\Omega}{4\pi}\,\frac{s}{s-\cos\theta} = \int_{-1}^{1}\frac{dx}{2}\,\frac{s}{s-x} = -\frac{s}{2}\ln|s-x|\Big|_{-1}^{1} = \frac{s}{2}\ln\left|\frac{s+1}{s-1}\right|$$

$$\mathrm{Im}\int \frac{d\Omega}{4\pi}\,\frac{-s}{s-\cos\theta+i\eta} = \frac{s}{2}\int_{-1}^{1} dx\,(-\pi\,\delta(s-x)) = +\frac{\pi s}{2}\,\theta(|s|<1)$$

$$\Rightarrow \quad \chi_0(q,\omega+i\eta) = N_0\left[1-\frac{S}{2}\ln\left|\frac{1+S}{1-S}\right|\right] + i\frac{\pi}{2}N_0 S\,\Theta(|S|<1).$$

RPA response $\quad \chi_{RPA}(q,\omega+i\eta) = \dfrac{\chi_0(q,\omega+i\eta)}{1+V(q)\,\chi_0(q,\omega+i\eta)}.$

☆ Static screening

$$\varepsilon(q,\omega) = 1 + v(q)\,\chi_0(q,\omega+i\eta)$$

$$\omega=0 \Rightarrow \varepsilon(q,0) = 1 + 2\cdot\frac{4\pi e^2}{q^2}\int\frac{d^3k}{(2\pi)^3}\frac{-n(\varepsilon_{k+q})+n(\varepsilon_k)}{\varepsilon_{k+q}-\varepsilon_k}$$

$$= 1 + 2\cdot\frac{4\pi e^2}{q^2}\int\frac{d^3k}{(2\pi)^3}\frac{n_f(\varepsilon_k)\times 2}{\varepsilon_{k+q}-\varepsilon_k} \qquad \boxed{\begin{array}{c}\vec{k}+\vec{q}\to-\vec{k}\\ \vec{k}\to-\vec{k}-\vec{q}\end{array}}$$

$$= 1 + \frac{4\pi e^2}{q^2}\int\frac{d^3k}{(2\pi)^3}\frac{4}{\frac{\hbar^2k_f^2}{2m}\left[2\frac{\vec{k}}{k_f}\cdot\frac{\vec{q}}{k_f}+\left(\frac{q}{k_f}\right)^2\right]}$$

$$= 1 + \frac{4\pi e^2}{q^2}\int\frac{k^2dk}{(2\pi)^3}\int_{-1}^{1}d\cos\theta\,\frac{4\cdot 2\pi}{\varepsilon_f\left[\frac{2kq\cos\theta}{k_f^2}+\left(\frac{q}{k_f}\right)^2\right]} \qquad \text{define } x=\frac{q}{2k_f}$$

$$= 1 + \frac{4\pi e^2}{q^2}\,\frac{k_f^3}{\varepsilon_f}\,\frac{1}{4\pi^2}\int_0^1 d\left(\frac{k}{k_f}\right)\left(\frac{k}{k_f}\right)^2\int_{-1}^{1}d\cos\theta\,\frac{1}{\left[\frac{k}{k_f}x\cos\theta+x^2\right]}$$

$$= 1 + \frac{4\pi e^2}{q^2}N_0\left[\frac{1}{2}+\frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|\right]$$

as $q\to 0 \quad \varepsilon(q) = 1+\dfrac{4\pi e^2}{q^2}N_0 \Rightarrow V(q) = \dfrac{V_0(q)}{\varepsilon(q)} = \dfrac{4\pi e^2}{q^2+(1/\lambda)^2}$

Thomas-Fermi $\quad V(r) = \dfrac{1}{r}e^{-\lambda r}, \quad \lambda = \left[4\pi e^2 N_0\right]^{1/2}$

$$\Rightarrow \lambda\cdot k_F = \frac{1}{\sqrt{4/\pi}}\,\frac{1}{\left[e^2k_F/\frac{\hbar^2k_F^2}{m}\cdot 2\right]^{1/2}} \sim \sqrt{E_K/E_{int}} \quad\Rightarrow\quad \boxed{1/\lambda \sim k_F}$$

★ Friedel oscillation,

$$\varepsilon(q,0) = 1 + \frac{\lambda^2}{q^2} S(x), \quad \text{where } S(x) = \frac{1}{2}\left[1 + \frac{1-x^2}{2x} \ln\left|\frac{1-x}{1+x}\right|\right]$$

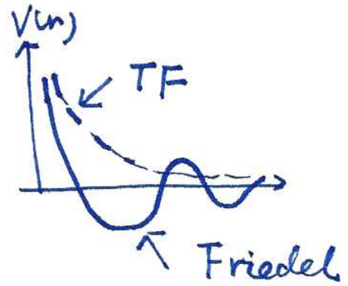
$$x = \frac{q}{2k_f}.$$

at $x = \frac{q}{2k_f} = 1$, $S(x)$ has a sudden drop $\leftarrow$ because $\varepsilon_{k+q} - \varepsilon_k > 0$ for all k if $q > 2k_f$.

$$V(r) = \int d^3\vec{q}\; e^{i\vec{q}\cdot\vec{r}} \frac{4\pi Z e^2}{q^2 + \lambda^2 S(q/2k_f)} \leftarrow$$

singular behavier at $x=1$.

as $r \to +\infty$, $V(r) \sim \text{const.} \frac{\cos 2k_f r}{r^3}$



★ Plasmon frequency at $s \gg 1$

$$1 + \frac{4\pi e^2}{q^2} \chi_0(q,\omega) = 0. \Rightarrow$$

The pole of $\chi(q,\omega)$, or, the zero of $\varepsilon(q,\omega)$, describes the intrinsic excitations.

why? It means even $V_{ex} = 0$, we still have responses.

at $s \gg 1$

$$\chi_0(q,\omega) = N_0\left[-\frac{1}{3s^2} - \frac{1}{5s^4}\right]$$

$$\varepsilon(q,\omega) = 1 + \frac{4\pi e^2 N_0}{q^2}\left[-\frac{1}{3s^2} - \frac{1}{5s^4}\right] = 0$$

$$\Rightarrow \frac{\omega^2}{\omega_p^2} = 1 + \frac{3}{10}\left(\frac{v_F q}{\omega_p}\right)^2 \leftarrow$$

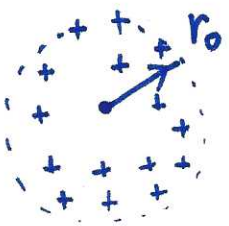
no-damping plasmon

☆ $$\delta \varepsilon_{HF}(k) \rightarrow -\sum_q n_{k+q} \frac{4\pi e^2}{q^2 + 4\pi e^2 \chi_0(q,0)}$$

☆ $\boxed{\text{Wigner crystal}}$

$$R_s = \frac{E_{int}}{E_K} = \frac{\frac{e^2}{d}}{\frac{\hbar^2}{md^2}} = \frac{d}{\frac{\hbar^2 e^2}{m}} \sim \frac{d}{a_0}$$

at $R_s >> 1$, perturbation picture does not apply. $\rightarrow$ Crystallization.

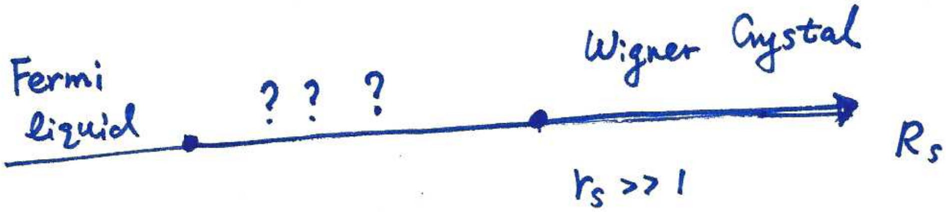


$$E\, 4\pi r^2 = 4\pi \cdot \frac{4\pi}{3} \rho r^3$$

$$E = \frac{4\pi}{3} \rho r = \frac{e}{r_0^3} r$$

$$F = eE = \frac{e^2}{r_0^3} r$$

$$\Rightarrow \boxed{\omega^2 = \frac{e^2}{m r_0^3} = \frac{e^2}{m(R_s a_0)^2} = \frac{1}{3}\omega_p^2}$$



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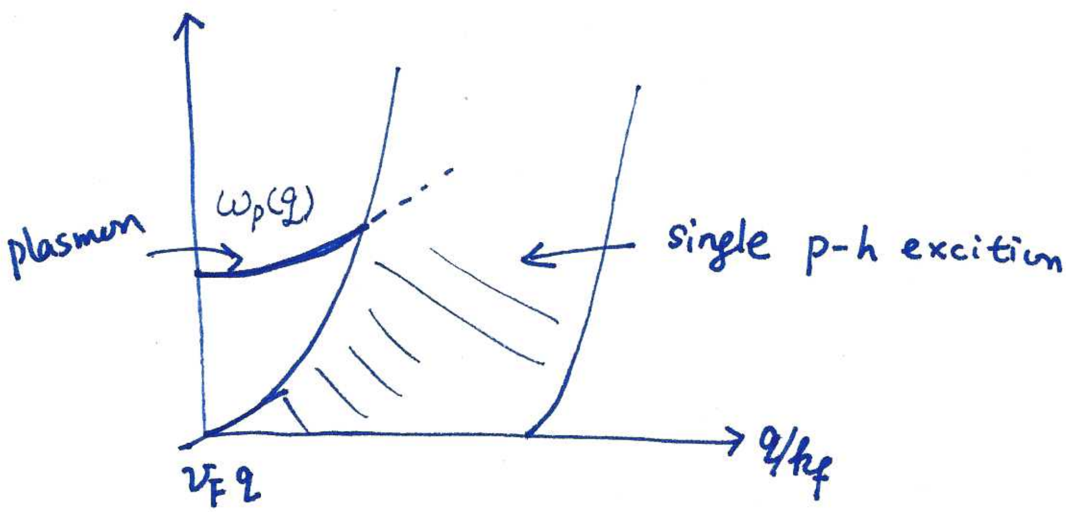

§ functional integral formalism

$$Z = \int D\bar{\psi} D\psi \; e^{-S}.$$

$$S = \int_0^\beta d\tau \sum_k \bar{\psi}(k,\tau)(\partial_\tau - \xi_k)\psi(k,\tau) + \frac{1}{2V}\sum_{q\neq 0}\frac{4\pi e^2}{q}\rho(q\tau)\rho(-q,\tau)$$

where $\rho(q) = \sum_{k\sigma} \bar{\psi}_\sigma(k,\tau)\psi_\sigma(k-q,\tau)$

The Hubbard - Stratonovich transformation

$$\exp\left[-\int_0^\beta d\tau \frac{1}{2V}\sum_{q\neq 0}\frac{4\pi e^2}{q^2}\rho(q,\tau)\rho(-q,\tau)\right]$$

$$= \int D\varphi(q,\tau) \exp\left[-\frac{1}{8\pi}\int_0^\beta d\tau \sum_{q\neq 0} q^2 \varphi(q\tau)\varphi(-q\tau)\right]$$

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$$\exp\left[-\int_0^\beta d\tau \frac{ie}{2\sqrt{V}}\sum_{q\neq 0}\varphi(q,\tau)\rho(-q,\tau) + \rho(q,\tau)\varphi(-q,\tau)\right]$$

then $Z = \int D\bar{\psi} D\psi D\varphi \; e^{-S(\bar{\psi}\psi\varphi)}$

$$S(\bar{\psi},\psi,\varphi) = \frac{1}{8\pi}\int_0^\beta d\tau \sum_{q\neq 0} q^2 \varphi(q,\tau)\varphi(-q,\tau)$$

$$+ \sum_k \bar{\psi}_\sigma(k,\tau)(\partial_\tau - \xi_k)\psi_\sigma(k,\tau) + \frac{ie}{2\sqrt{V}}\sum_{q\neq 0}\left(\varphi(q,\tau)\rho(-q,\tau) + \rho(q\tau)\varphi(-q,\tau)\right)$$

$$\frac{ie}{\sqrt{V}}\sum_{k,q}\bar{\psi}_\sigma(k,\tau)\left[\varphi(-q,\tau)\right]\psi_\sigma(k-q,\tau)$$

transform back to real space $\varphi(r,\tau) = \frac{1}{\sqrt{V}} \sum_q e^{i\vec{q}\cdot\vec{r}} \varphi(q,\tau)$

$$\Rightarrow S(\bar{\psi},\psi,\varphi) = -\int_0^\beta d\tau \int dr \frac{1}{8\pi}(\nabla\varphi)^2 + \bar{\psi}_\sigma(r,\tau)\left[\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu + ie\varphi(r,\tau)\right]\psi_\sigma(r,\tau)$$

Integrate out fermions $\Rightarrow$

$$Z = \int D\varphi \exp\left[-\int_0^\beta d\tau \int dr \frac{1}{8\pi}(\nabla\varphi)^2\right] \det\left[\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu + ie\varphi(r,\tau)\right].$$

Remark: The physical meaning of $\varphi(r,\tau)$ is not clear. Naively the saddle point equation $\varphi(r,\tau) \sim \left\langle \int iV(r-r')\rho(r')dr' \right\rangle$, but the mean field hamiltonian is no-hermitian: $-\frac{\hbar^2}{2m}\nabla^2 - \mu + ie\varphi$, such that the average of $\left\langle i\int V(r-r')\rho(r')dr' \right\rangle$ can still be real. We may further think what does it really mean.

The determinaint is defined in the basis of $\varphi(r,\tau)$, let's transform to $(k, i\omega_n)$ space, according to the Fourier transform

$$\varphi(r,\tau) = \frac{1}{(\beta V)^{1/2}} \sum_q \sum_l e^{i\vec{q}\cdot\vec{r} - i\omega_l\tau} \varphi(q,\omega_l)$$

then

$$\left[\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu + ie\varphi(r,\tau)\right]_{(k\omega_n,\, k'\omega_n')}$$

$$= \int dr d\tau \int dr' d\tau' \; \langle k\omega_n | r\tau \rangle \left[\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu + ie\varphi(r,\tau) \right]_{r\tau, r'\tau'} \langle r'\tau' | k'\omega_n' \rangle$$

$$= \int dr d\tau \; \frac{e^{-i(\vec{k}\cdot\vec{r} - \omega_n \tau)}}{\sqrt{\beta V}} \left[\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu + ie\varphi(r,\tau) \right] \frac{e^{i(k'\cdot r - \omega_n' \tau)}}{\sqrt{\beta V}}$$

$$= \Big[\underbrace{-i\omega_n + \frac{\hbar^2}{2m}k^2 - \mu}_{\xi_k} \Big] \delta_{k,k'} \delta_{\omega_n, \omega_n'} + \frac{ie}{\sqrt{\beta V}} \varphi(k-k', \omega_n - \omega_n')$$

$\omega_n = \frac{2\pi n}{\beta}$ (bosonic frequency)

write down

$$\boxed{\begin{aligned} M_{k\omega_n, k'\omega_n'} &= (M_0)_{k\omega_n, k'\omega_n'} + (M_1)_{k\omega_n, k'\omega_n'} \\ &= -\mathcal{G}_0^{-1}(k\, i\omega_n)\, \delta_{k\omega_n, k'\omega_n'} + \frac{ie}{(\beta V)^{1/2}} \varphi(k-k', \omega_n - \omega_n') \end{aligned}}$$

then $\mathcal{Z} = \int D\varphi \; e^{-S_{eff}(\varphi)}$, with $S_{eff}(\varphi) = \int_0^\beta d\tau \int dr \frac{1}{8\pi} \left(\nabla\varphi(r,\tau)\right)^2$

$- 2 \ln \det M.$

spin degeneracy

$$\boxed{\ln \det M = \mathrm{tr} \ln M = \mathrm{tr} \ln (M_0 + M_1)}$$

$$\ln(M_0 + M_1) = \ln M_0 + \ln(1 + M_0^{-1} M_1) = \ln M_0 + \ln(1 - \mathcal{G}_0 M_1)$$

$$= \ln M_0 - \sum_{n=1}^{\infty} \frac{1}{n} \left(\mathcal{G}_0 M_1\right)^n.$$ only M_1 contains φ-field

$$\Rightarrow \mathcal{Z} = \int D\varphi \; e^{-\left\{ \int_0^\beta d\tau \int dr \frac{1}{8\pi} (\nabla\varphi(r,\tau))^2 - \sum_{n=1}^{\infty} \frac{1}{n} \mathrm{tr} [\mathcal{G}_0 M_1]^n \right.}.$$

① $n=1$: $tr[\mathcal{G}_0 M_1] = \sum_{kk'} (\mathcal{G}_0)_{kk'} (M_1)_{k'k} = \sum_k \mathcal{G}_0(k) M_{1,kk}$

$$= \sum_k G_0(k) \left(\frac{ie}{(\beta V)^{1/2}} \varphi(0) \right)$$

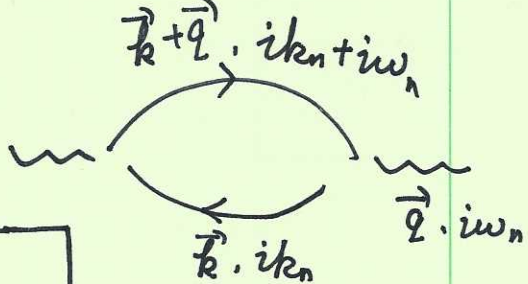
we set $\varphi(0) = 0$. $\varphi(0) \sim V(q=0)\,\rho(q=0)$ which is proportional the overall particle density. Set $\underbrace{\varphi(0)}_{=0}$ to neutralize the background.

② Gaussian fluctuation

$$tr[(\mathcal{G}_0 M_1)^2] = \sum_{kk'} \mathcal{G}_0(k) (M_1)_{kk'} \mathcal{G}_0(k') (M_1)_{k'k}$$

$$= \frac{1}{2} \sum_q \frac{e^2}{\beta V} \left(2 \sum_k \mathcal{G}_0(k) \mathcal{G}_0(k+q) \right) \varphi(q) \varphi(-q)$$

define $\pi(q) = \frac{2}{\beta V} \sum_k \mathcal{G}_0(k) \mathcal{G}_0(k+q)$



$$\Rightarrow \boxed{S_{eff} = \frac{1}{2} \sum_q \left[\frac{\vec{q}^2}{4\pi} - e^2 \pi(\vec{q}, iq_n) \right] \varphi(q) \varphi(-q)}$$

vaccum polarization

This $\pi(\vec{q}, iq_n)$ is basically $-\chi^0(\vec{q}, iq_n)$ we calculated before. $\Rightarrow$ $\boxed{\text{Gaussian fluctuation} \equiv \text{RPA approxiation}}$